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rac-(*E,E*)-*N,N'*-Bis(2-chlorobenzylidene)-cyclohexane-1,2-diamine

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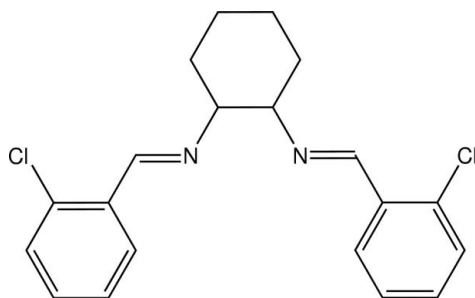
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 Key indicators: single-crystal X-ray study; *T* = 293 K; mean $\sigma(\text{C}-\text{C})$ = 0.004 Å; *R* factor = 0.046; *wR* factor = 0.106; data-to-parameter ratio = 15.1.

In the title racemic Schiff base ligand, C₂₀H₂₀Cl₂N₂, which was prepared by the condensation of 2-chlorobenzaldehyde and cyclohexane-1,2-diamine, the cyclohexane ring adopts a chair conformation and the dihedral angle between the aromatic rings of the 2-chlorophenyl substituent groups is 62.52 (8)°. In the structure, there are two short intramolecular methine C—H...Cl interactions [C...Cl = 3.066 (2) and 3.076 (3) Å], and in the crystal there are also weak intermolecular aromatic C—H...Cl [3.464 (3), 3.553 (3) and 3.600 (3) Å] and Cl...Cl [3.557 (3) and 3.891 (3) Å] contacts.

Related literature

For the crystal structures of some Schiff bases derived from cyclohexane-1,2-diamine, see: Arvinnezhad *et al.* (2012); Fan *et al.* (2011); Saleh Salga *et al.* (2010). For applications of chiral Schiff base ligands, see: Da Silva *et al.* (2011); Dhar & Taploo (1982); Przybylski *et al.* (2009); Gupta & Sutar (2008). For the synthesis of the title compound, see: Larrow & Jacobsen (1998).



Experimental

Crystal data

 C₂₀H₂₀Cl₂N₂
M_r = 359.28

 Monoclinic, *P*2₁/*n*
a = 5.9029 (5) Å

b = 19.5613 (13) Å

c = 16.1662 (11) Å

β = 93.493 (7)°

V = 1863.2 (2) Å³
Z = 4

 Mo *K*α radiation

 μ = 0.35 mm⁻¹
T = 293 K

0.30 × 0.20 × 0.15 mm

Data collection

Agilent Xcalibur Eos diffractometer

Absorption correction: multi-scan

 (*CrysAlis PRO*; Agilent, 2011)

T_{min} = 0.902, *T_{max}* = 0.949

7483 measured reflections

3273 independent reflections

 2252 reflections with *I* > 2σ(*I*)

R_{int} = 0.030

Refinement

R[*F*² > 2σ(*F*²)] = 0.046

wR(*F*²) = 0.106

S = 1.02

3273 reflections

217 parameters

H-atom parameters constrained

 Δρ_{max} = 0.28 e Å⁻³

 Δρ_{min} = -0.20 e Å⁻³

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2261).

References

- Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
- Arvinnezhad, H., Jadidi, K. & Notash, B. (2012). *Acta Cryst.* **E68**, o407–o408.
- Burnett, M. N. & Johnson, C. K. (1996). *ORTEP III*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Da Silva, C. M., Da Silva, D. L., Modolo, L. V., Alves, R. B., De Resende, M. A., Martins, C. V. B. & De Faetima, A. (2011). *J. Adv. Res.* **2**, 1–8.
- Dhar, D. N. & Taploo, C. L. (1982). *J. Sci. Ind. Res.* **41**, 501–506.
- Fan, P., Ge, C., Zhang, X., Zhang, R. & Li, S. (2011). *Acta Cryst.* **E67**, o3399.
- Gupta, K. C. & Sutar, A. K. (2008). *Coord. Chem. Rev.* **252**, 1420–1450.
- Larrow, J. F. & Jacobsen, E. N. (1998). *Org. Synth.* **75**, 1–11.
- Przybylski, P., Huczynski, A., Pyta, K., Brzezinski, B. & Bartl, F. (2009). *Curr. Org. Chem.* **13**, 124–148.
- Saleh Salga, M., Khaleedi, H., Mohd Ali, H. & Puteh, R. (2010). *Acta Cryst.* **E66**, o1095.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2013). E69, o1075 [doi:10.1107/S1600536813014554]

rac*-(*E,E*)-*N,N'*-Bis(2-chlorobenzylidene)cyclohexane-1,2-diamine*Ismail Warad, Mousa Al-Noaimi, Salim F. Haddad, Yasmin Al-Demeri and Belkheir Hammouti****Comment**

The chelating chiral Schiff bases are significant compounds in chemistry so that several reviews have been published on these substances (Gupta & Sutar, 2008; Da Silva *et al.*, 2011; Przybylski *et al.*, 2009). Because of their stereochemical features, as well as their industrial properties (Dhar & Taploo, 1982) and potent biological activities (Da Silva *et al.*, 2011; Przybylski *et al.*, 2009), they are very attractive synthetic targets. Furthermore, it should be stressed that these useful and recyclable chemicals have been widely used in various enantioselective reactions, such as cyclopropanation, aziridination, epoxidation or the Diels–Alder reaction, and as ligands or catalysts.

The title Schiff base, C₂₀H₂₀Cl₂N₂, was prepared by condensation of commercially available 2-chlorobenzaldehyde and (*1R,2R*)-diaminocyclohexane and the structure is reported herein. However, this compound is racemic, in which the cyclohexane ring adopts the expected chair conformation, with a dihedral angle of 62.52 (8)° between the aromatic rings of the two 2-chlorophenyl substituent groups (Fig. 1). The structure of the chiral isomeric (*1R,2R*) 4-chlorophenyl analogue has been reported (Arvinnezhad *et al.*, 2012). In the title compound, the conformation is stabilized by intramolecular C7—H···C11 and C14—H···Cl2 interactions [3.066 (2) and 3.076 (3) Å, respectively] (Table 1). In the crystal there are weak intermolecular methine C—H···Cl interactions [C10—H···Cl1 [3.600 (3) Å] (−*x* + 2, −*y*, −*z*), C11—H···Cl1 [3.553 (3) Å] (*x* − 1, *y*, *z*) and C20—H···Cl2 [3.464 (3) Å] (1 + *x* + 1, *y*, *z*)]. Also present in the crystal are Cl···Cl contacts [Cl1···Cl1, 3.557 (3) Å (−*x* + 1, −*y*, −*z*)] and 3.891 (3) Å (−*x* + 2, −*y*, −*z*) (Fig. 2).

Experimental

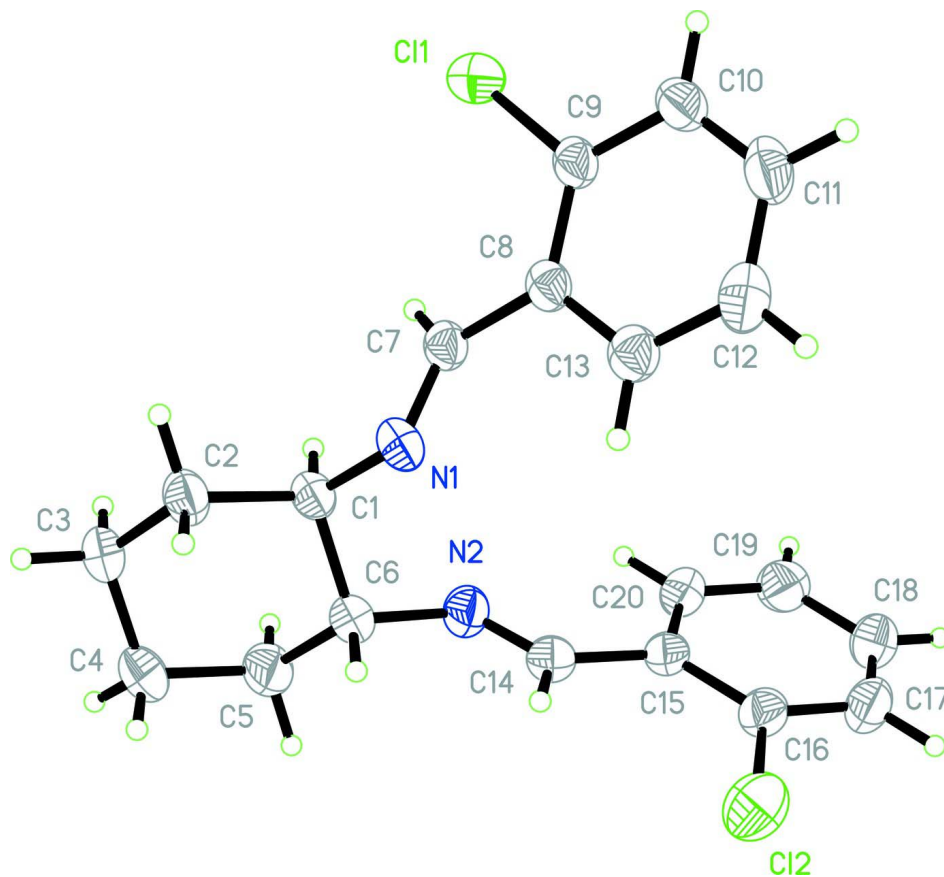
(*R,R*)-1,2-Diaminocyclohexane (1 g, 8.9 mmol) was dissolved in EtOH (10 ml) and the mixture was stirred and heated gently (50 °C) for 10 min, after which a solution of 2-chlorobenzaldehyde (2.6 g, 18 mmol, 2 equivalents) in EtOH (5 ml) was added dropwise. The stirred reaction mixture was refluxed for a period of 4 h, with the reaction progress monitored by thin-layer chromatography. Upon completion of the reaction, the mixture was cooled to room temperature and the solid obtained was filtered off, washed with cold water and crystallized from ethanol (95%), with a 85% yield.

Refinement

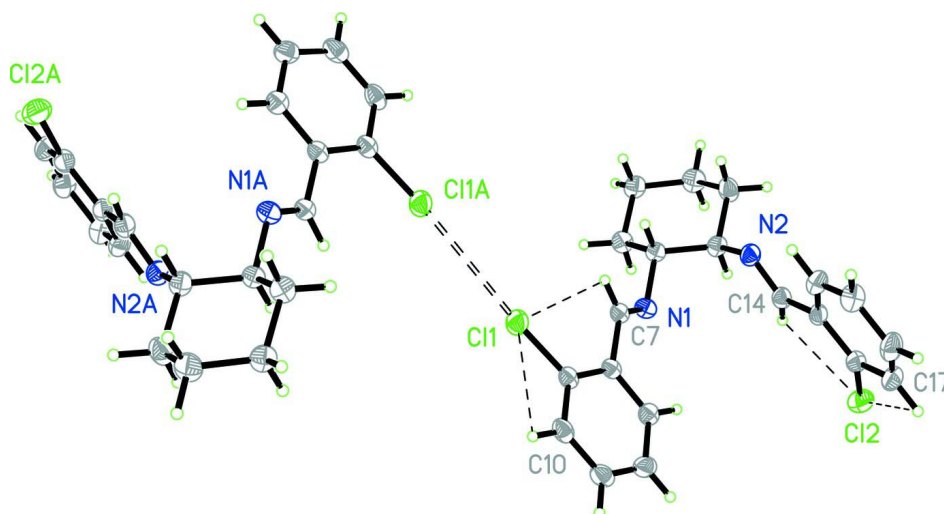
H atoms were positioned geometrically with C—H = 0.93 Å (aromatic), 0.97 Å (methylene) or 0.98 Å (methine) and allowed to ride in the refinement, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The largest difference peak and hole are 0.276 and −0.204 e Å^{−3}.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

**Figure 1**

Molecular conformation and atom-numbering scheme for the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

**Figure 2**

Molecular conformation showing intramolecular C7—H...Cl1, C10—H...Cl1, C14—H...Cl2 and C17—H...Cl2 contacts, as well as a short intermolecular Cl1...Cl1A contact. For symmetry code (A): $-x + 1, -y, -z$.

rac-(*E,E*)-*N,N'*-Bis(2-chlorobenzylidene)cyclohexane-1,2-diamine

Crystal data

| | |
|--------------------------------|---|
| $C_{20}H_{20}Cl_2N_2$ | $F(000) = 752$ |
| $M_r = 359.28$ | $D_x = 1.281 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: $-P 2_1n$ | Cell parameters from 2442 reflections |
| $a = 5.9029 (5) \text{ \AA}$ | $\theta = 3.1\text{--}29.1^\circ$ |
| $b = 19.5613 (13) \text{ \AA}$ | $\mu = 0.35 \text{ mm}^{-1}$ |
| $c = 16.1662 (11) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $\beta = 93.493 (7)^\circ$ | Block, colourless |
| $V = 1863.2 (2) \text{ \AA}^3$ | $0.30 \times 0.20 \times 0.15 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|--|--|
| Agilent Xcalibur Eos diffractometer | 7483 measured reflections |
| Radiation source: Enhance (Mo) X-ray Source | 3273 independent reflections |
| Graphite monochromator | 2252 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $16.0534 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.030$ |
| ω scans | $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 3.3^\circ$ |
| Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2011) | $h = -7 \rightarrow 6$ |
| $T_{\text{min}} = 0.902$, $T_{\text{max}} = 0.949$ | $k = -23 \rightarrow 18$ |
| | $l = -19 \rightarrow 17$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | H-atom parameters constrained |
| $wR(F^2) = 0.106$ | $w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.4202P]$ |
| $S = 1.02$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3273 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 217 parameters | $\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| Cl1 | 0.73684 (13) | 0.05324 (3) | 0.02770 (4) | 0.0762 (2) |
| Cl2 | 1.12436 (13) | 0.46542 (4) | 0.17646 (5) | 0.0914 (3) |
| N1 | 0.7836 (3) | 0.26396 (10) | -0.03727 (11) | 0.0555 (5) |
| C8 | 0.9564 (4) | 0.17516 (12) | 0.04725 (12) | 0.0489 (6) |

| | | | | |
|------|------------|--------------|---------------|------------|
| C1 | 0.5739 (4) | 0.29405 (11) | -0.07382 (12) | 0.0520 (6) |
| H1B | 0.4442 | 0.2674 | -0.0567 | 0.062* |
| C6 | 0.5559 (4) | 0.36693 (12) | -0.04157 (13) | 0.0583 (7) |
| H6A | 0.6885 | 0.3932 | -0.0568 | 0.070* |
| N2 | 0.5510 (4) | 0.36480 (10) | 0.04896 (11) | 0.0613 (6) |
| C14 | 0.7170 (5) | 0.39062 (12) | 0.09007 (14) | 0.0586 (6) |
| H14A | 0.8318 | 0.4110 | 0.0617 | 0.070* |
| C7 | 0.7660 (4) | 0.20790 (12) | -0.00033 (12) | 0.0492 (6) |
| H7A | 0.6258 | 0.1861 | -0.0032 | 0.059* |
| C13 | 1.1395 (4) | 0.21396 (13) | 0.07903 (13) | 0.0587 (6) |
| H13A | 1.1465 | 0.2602 | 0.0661 | 0.070* |
| C15 | 0.7373 (4) | 0.38992 (12) | 0.18143 (14) | 0.0550 (6) |
| C10 | 1.1237 (5) | 0.07662 (14) | 0.11857 (14) | 0.0673 (8) |
| H10A | 1.1179 | 0.0304 | 0.1317 | 0.081* |
| C9 | 0.9546 (4) | 0.10611 (12) | 0.06799 (12) | 0.0540 (6) |
| C16 | 0.9153 (4) | 0.42153 (12) | 0.22641 (15) | 0.0615 (7) |
| C20 | 0.5769 (5) | 0.35715 (13) | 0.22604 (15) | 0.0669 (7) |
| H20A | 0.4546 | 0.3359 | 0.1976 | 0.080* |
| C11 | 1.3010 (5) | 0.11644 (17) | 0.14930 (15) | 0.0777 (9) |
| H11A | 1.4156 | 0.0972 | 0.1838 | 0.093* |
| C17 | 0.9323 (5) | 0.42009 (15) | 0.31214 (17) | 0.0756 (8) |
| H17A | 1.0535 | 0.4415 | 0.3411 | 0.091* |
| C2 | 0.5740 (4) | 0.29389 (13) | -0.16818 (13) | 0.0634 (7) |
| H2B | 0.7073 | 0.3178 | -0.1853 | 0.076* |
| H2C | 0.5804 | 0.2472 | -0.1880 | 0.076* |
| C3 | 0.3615 (5) | 0.32848 (13) | -0.20597 (14) | 0.0679 (7) |
| H3A | 0.3679 | 0.3298 | -0.2658 | 0.081* |
| H3B | 0.2292 | 0.3020 | -0.1931 | 0.081* |
| C5 | 0.3413 (5) | 0.40078 (14) | -0.07892 (15) | 0.0783 (9) |
| H5A | 0.3340 | 0.4476 | -0.0594 | 0.094* |
| H5B | 0.2093 | 0.3766 | -0.0610 | 0.094* |
| C12 | 1.3100 (4) | 0.18501 (17) | 0.12915 (15) | 0.0725 (8) |
| H12A | 1.4315 | 0.2116 | 0.1495 | 0.087* |
| C19 | 0.5930 (5) | 0.35511 (14) | 0.31149 (17) | 0.0783 (8) |
| H19A | 0.4841 | 0.3322 | 0.3401 | 0.094* |
| C4 | 0.3382 (5) | 0.40022 (14) | -0.17353 (16) | 0.0825 (9) |
| H4A | 0.1970 | 0.4199 | -0.1962 | 0.099* |
| H4B | 0.4620 | 0.4281 | -0.1915 | 0.099* |
| C18 | 0.7716 (6) | 0.38728 (15) | 0.35396 (17) | 0.0819 (9) |
| H18A | 0.7825 | 0.3866 | 0.4116 | 0.098* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| Cl1 | 0.0871 (5) | 0.0566 (4) | 0.0835 (5) | 0.0021 (4) | -0.0058 (4) | 0.0000 (3) |
| Cl2 | 0.0686 (5) | 0.1026 (6) | 0.1027 (6) | -0.0136 (4) | 0.0018 (4) | -0.0098 (4) |
| N1 | 0.0581 (13) | 0.0600 (13) | 0.0482 (11) | 0.0065 (10) | 0.0025 (10) | 0.0112 (9) |
| C8 | 0.0547 (15) | 0.0576 (15) | 0.0350 (11) | 0.0102 (12) | 0.0076 (10) | -0.0003 (10) |
| C1 | 0.0560 (15) | 0.0538 (14) | 0.0457 (12) | 0.0028 (12) | 0.0003 (11) | 0.0077 (10) |
| C6 | 0.0690 (17) | 0.0549 (15) | 0.0499 (13) | 0.0001 (13) | -0.0050 (12) | 0.0039 (11) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| N2 | 0.0686 (14) | 0.0649 (13) | 0.0497 (11) | 0.0024 (11) | -0.0019 (10) | -0.0047 (9) |
| C14 | 0.0677 (17) | 0.0493 (14) | 0.0583 (15) | 0.0044 (13) | 0.0002 (13) | -0.0018 (11) |
| C7 | 0.0542 (14) | 0.0543 (14) | 0.0393 (11) | 0.0055 (12) | 0.0034 (10) | -0.0002 (11) |
| C13 | 0.0649 (17) | 0.0636 (16) | 0.0478 (13) | 0.0032 (13) | 0.0052 (12) | -0.0007 (11) |
| C15 | 0.0638 (16) | 0.0454 (14) | 0.0547 (14) | 0.0065 (12) | -0.0065 (13) | -0.0056 (11) |
| C10 | 0.087 (2) | 0.0641 (17) | 0.0496 (14) | 0.0270 (16) | -0.0021 (14) | -0.0012 (12) |
| C9 | 0.0653 (16) | 0.0589 (15) | 0.0376 (12) | 0.0145 (13) | 0.0024 (11) | -0.0025 (10) |
| C16 | 0.0647 (17) | 0.0533 (15) | 0.0656 (16) | 0.0062 (13) | -0.0041 (13) | -0.0067 (12) |
| C20 | 0.0782 (19) | 0.0636 (17) | 0.0576 (16) | -0.0079 (15) | -0.0060 (14) | -0.0053 (12) |
| C11 | 0.081 (2) | 0.097 (2) | 0.0536 (15) | 0.0358 (18) | -0.0137 (15) | -0.0084 (15) |
| C17 | 0.081 (2) | 0.076 (2) | 0.0680 (18) | 0.0003 (17) | -0.0157 (16) | -0.0181 (15) |
| C2 | 0.0752 (18) | 0.0686 (17) | 0.0461 (13) | 0.0056 (14) | 0.0021 (13) | 0.0066 (12) |
| C3 | 0.0817 (19) | 0.0721 (18) | 0.0481 (14) | 0.0024 (15) | -0.0103 (13) | 0.0079 (12) |
| C5 | 0.096 (2) | 0.0648 (17) | 0.0712 (18) | 0.0260 (16) | -0.0146 (16) | -0.0042 (14) |
| C12 | 0.0621 (17) | 0.098 (2) | 0.0570 (16) | 0.0101 (17) | -0.0040 (14) | -0.0143 (15) |
| C19 | 0.095 (2) | 0.0727 (19) | 0.0674 (18) | -0.0071 (17) | 0.0074 (16) | 0.0016 (14) |
| C4 | 0.100 (2) | 0.0716 (19) | 0.0717 (18) | 0.0166 (17) | -0.0243 (17) | 0.0146 (14) |
| C18 | 0.111 (3) | 0.077 (2) | 0.0552 (16) | 0.0005 (19) | -0.0075 (18) | -0.0097 (14) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|--------------|-----------|
| C11—C9 | 1.745 (2) | C10—H10A | 0.9300 |
| C12—C16 | 1.742 (3) | C16—C17 | 1.384 (3) |
| N1—C7 | 1.256 (3) | C20—C19 | 1.379 (3) |
| N1—C1 | 1.462 (3) | C20—H20A | 0.9300 |
| C8—C9 | 1.392 (3) | C11—C12 | 1.382 (4) |
| C8—C13 | 1.393 (3) | C11—H11A | 0.9300 |
| C8—C7 | 1.469 (3) | C17—C18 | 1.359 (4) |
| C1—C6 | 1.524 (3) | C17—H17A | 0.9300 |
| C1—C2 | 1.525 (3) | C2—C3 | 1.520 (3) |
| C1—H1B | 0.9800 | C2—H2B | 0.9700 |
| C6—N2 | 1.466 (3) | C2—H2C | 0.9700 |
| C6—C5 | 1.522 (3) | C3—C4 | 1.507 (4) |
| C6—H6A | 0.9800 | C3—H3A | 0.9700 |
| N2—C14 | 1.256 (3) | C3—H3B | 0.9700 |
| C14—C15 | 1.475 (3) | C5—C4 | 1.529 (3) |
| C14—H14A | 0.9300 | C5—H5A | 0.9700 |
| C7—H7A | 0.9300 | C5—H5B | 0.9700 |
| C13—C12 | 1.375 (3) | C12—H12A | 0.9300 |
| C13—H13A | 0.9300 | C19—C18 | 1.375 (4) |
| C15—C20 | 1.383 (3) | C19—H19A | 0.9300 |
| C15—C16 | 1.386 (3) | C4—H4A | 0.9700 |
| C10—C11 | 1.373 (4) | C4—H4B | 0.9700 |
| C10—C9 | 1.378 (3) | C18—H18A | 0.9300 |
| C7—N1—C1 | 116.8 (2) | C15—C20—H20A | 119.1 |
| C9—C8—C13 | 117.2 (2) | C10—C11—C12 | 120.3 (2) |
| C9—C8—C7 | 122.2 (2) | C10—C11—H11A | 119.9 |
| C13—C8—C7 | 120.5 (2) | C12—C11—H11A | 119.9 |
| N1—C1—C6 | 108.26 (18) | C18—C17—C16 | 119.8 (3) |

| | | | |
|---------------|--------------|-----------------|--------------|
| N1—C1—C2 | 110.58 (19) | C18—C17—H17A | 120.1 |
| C6—C1—C2 | 110.38 (18) | C16—C17—H17A | 120.1 |
| N1—C1—H1B | 109.2 | C3—C2—C1 | 110.5 (2) |
| C6—C1—H1B | 109.2 | C3—C2—H2B | 109.5 |
| C2—C1—H1B | 109.2 | C1—C2—H2B | 109.5 |
| N2—C6—C5 | 110.0 (2) | C3—C2—H2C | 109.5 |
| N2—C6—C1 | 108.72 (18) | C1—C2—H2C | 109.5 |
| C5—C6—C1 | 110.19 (19) | H2B—C2—H2C | 108.1 |
| N2—C6—H6A | 109.3 | C4—C3—C2 | 111.4 (2) |
| C5—C6—H6A | 109.3 | C4—C3—H3A | 109.3 |
| C1—C6—H6A | 109.3 | C2—C3—H3A | 109.3 |
| C14—N2—C6 | 117.0 (2) | C4—C3—H3B | 109.3 |
| N2—C14—C15 | 122.6 (3) | C2—C3—H3B | 109.3 |
| N2—C14—H14A | 118.7 | H3A—C3—H3B | 108.0 |
| C15—C14—H14A | 118.7 | C6—C5—C4 | 110.7 (2) |
| N1—C7—C8 | 123.1 (2) | C6—C5—H5A | 109.5 |
| N1—C7—H7A | 118.4 | C4—C5—H5A | 109.5 |
| C8—C7—H7A | 118.4 | C6—C5—H5B | 109.5 |
| C12—C13—C8 | 121.1 (3) | C4—C5—H5B | 109.5 |
| C12—C13—H13A | 119.5 | H5A—C5—H5B | 108.1 |
| C8—C13—H13A | 119.5 | C13—C12—C11 | 120.1 (3) |
| C20—C15—C16 | 117.0 (2) | C13—C12—H12A | 119.9 |
| C20—C15—C14 | 120.7 (2) | C11—C12—H12A | 119.9 |
| C16—C15—C14 | 122.3 (3) | C18—C19—C20 | 119.4 (3) |
| C11—C10—C9 | 119.1 (3) | C18—C19—H19A | 120.3 |
| C11—C10—H10A | 120.5 | C20—C19—H19A | 120.3 |
| C9—C10—H10A | 120.5 | C3—C4—C5 | 111.0 (2) |
| C10—C9—C8 | 122.2 (2) | C3—C4—H4A | 109.4 |
| C10—C9—C11 | 117.6 (2) | C5—C4—H4A | 109.4 |
| C8—C9—C11 | 120.09 (17) | C3—C4—H4B | 109.4 |
| C17—C16—C15 | 121.5 (3) | C5—C4—H4B | 109.4 |
| C17—C16—C12 | 117.6 (2) | H4A—C4—H4B | 108.0 |
| C15—C16—C12 | 120.8 (2) | C17—C18—C19 | 120.3 (3) |
| C19—C20—C15 | 121.9 (2) | C17—C18—H18A | 119.8 |
| C19—C20—H20A | 119.1 | C19—C18—H18A | 119.8 |
| | | | |
| C7—N1—C1—C6 | 126.4 (2) | C20—C15—C16—C17 | 0.3 (4) |
| C7—N1—C1—C2 | -112.5 (2) | C14—C15—C16—C17 | -179.7 (2) |
| N1—C1—C6—N2 | -60.1 (3) | C20—C15—C16—C12 | -178.99 (19) |
| C2—C1—C6—N2 | 178.69 (19) | C14—C15—C16—C12 | 1.0 (3) |
| N1—C1—C6—C5 | 179.2 (2) | C16—C15—C20—C19 | -0.7 (4) |
| C2—C1—C6—C5 | 58.1 (3) | C14—C15—C20—C19 | 179.3 (2) |
| C5—C6—N2—C14 | -125.3 (2) | C9—C10—C11—C12 | -0.5 (4) |
| C1—C6—N2—C14 | 114.0 (2) | C15—C16—C17—C18 | -0.2 (4) |
| C6—N2—C14—C15 | -178.0 (2) | C12—C16—C17—C18 | 179.1 (2) |
| C1—N1—C7—C8 | -173.03 (19) | N1—C1—C2—C3 | -177.1 (2) |
| C9—C8—C7—N1 | -161.7 (2) | C6—C1—C2—C3 | -57.3 (3) |
| C13—C8—C7—N1 | 23.4 (3) | C1—C2—C3—C4 | 56.3 (3) |
| C9—C8—C13—C12 | -0.4 (3) | N2—C6—C5—C4 | -177.2 (2) |

| | | | |
|----------------|--------------|-----------------|-----------|
| C7—C8—C13—C12 | 174.8 (2) | C1—C6—C5—C4 | -57.3 (3) |
| N2—C14—C15—C20 | 3.3 (4) | C8—C13—C12—C11 | -0.4 (4) |
| N2—C14—C15—C16 | -176.7 (2) | C10—C11—C12—C13 | 0.9 (4) |
| C11—C10—C9—C8 | -0.4 (4) | C15—C20—C19—C18 | 0.9 (4) |
| C11—C10—C9—C11 | 178.1 (2) | C2—C3—C4—C5 | -55.8 (3) |
| C13—C8—C9—C10 | 0.8 (3) | C6—C5—C4—C3 | 56.3 (3) |
| C7—C8—C9—C10 | -174.3 (2) | C16—C17—C18—C19 | 0.5 (4) |
| C13—C8—C9—C11 | -177.66 (17) | C20—C19—C18—C17 | -0.8 (4) |
| C7—C8—C9—C11 | 7.3 (3) | | |

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|----------------|------------|--------------|--------------|----------------|
| C7—H7A...C11 | 0.93 | 2.72 | 3.066 (2) | 103 |
| C14—H14A...C12 | 0.93 | 2.68 | 3.076 (3) | 107 |